Computational Physics

Lecture-04

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- Basis Concepts
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Numerical Differentiation

- First order derivative

$$f_i^{(1)} \approx \frac{f_{i+1} - f_i}{h} + \mathrm{O}(h)$$ Forward

$$f_i^{(1)} \approx \frac{f_{i+1} - f_{i-1}}{2h} + \mathrm{O}(h^2)$$ Central

$$f_i^{(1)} \approx \frac{f_i - f_{i-1}}{h} + \mathrm{O}(h)$$ Backward

x	$f(x)$	$f^{(1)}(x)$
x_0	f_0	$f_0^{(1)}$
x_1	f_1	$f_1^{(1)}$
x_2	f_2	$f_2^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(1)}$
x_i	f_i	$f_i^{(1)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(1)}$
x_N	f_N	$f_N^{(1)}$

Numerical Differentiation

- Second order derivative

$$f_i^{(2)} \approx \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} + \mathrm{O}(h)$$ Forward

$$f_i^{(2)} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + \mathrm{O}(h^2)$$ Central

$$f_i^{(2)} \approx \frac{f_{i-2} - 2f_{i-1} + f_i}{h^2} + \mathrm{O}(h)$$ Backward

x	$f(x)$	$f^{(2)}(x)$
x_0	f_0	$f_0^{(2)}$
x_1	f_1	$f_1^{(2)}$
x_2	f_2	$f_2^{(2)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(2)}$
x_i	f_i	$f_i^{(2)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(2)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(2)}$
x_N	f_N	$f_N^{(2)}$